Microscopy reveals secret of beryl's iron heart

Discovery of metal-stuffed channels in mineral family points way to tuning the material's colour

Beryllium is named for its most celebrated natural manifestation: the mineral beryl (beryllium aluminosilicate), of which emerald is one of the gem-like forms. Beryl containing trace amounts of iron, however, constitutes the cyan gemstone aquamarine and the golden-hued heliodor – the 'gift of the sun'. Yet despite these illustrious forms, beryl still holds secrets.

One has now been teased out by scanning transmission electron microscopy (Stem), which reveals that channels in the crystal structure made from rings of silicate tetrahedra can host metal atoms. To obtain these results, Bodil Holst of the University of Bergen in Norway and her colleagues have used a technique called *Z*-contrast imaging, which collects electrons scattered through large angles to improve the contrast and resolution. The work supplies the first direct evidence for the long suspected occupancy of the mineral's channels.[1]

'People have speculated that there might be metal atoms in the channels,' says Holst, but there was no evidence. In cross sections of a heliodor sample, she and her co-workers see bright spots in the 0.5nm wide pores that they think are most probably iron atoms. 'The typical alkali ions present in beryl crystals are either too small (like lithium) or present in too small an amount to explain the fuzzy dots,' says Holst. 'The only element which, according to mass spectrometry, was present in sufficient amounts and had a mass big enough to give this contrast is iron.' The researchers estimate that there is likely to be about one iron atom for every 35 channels in each atomic plane.

It's not clear whether the channel atoms contribute to the colour that makes some forms of beryl so desirable. 'There are speculations, but we just don't know, and they might not contribute at all,' says Holst.

The fact that atoms can get into the channels at all might point to applications. By inserting atoms or molecules selectively, says Holst, we 'can potentially design new materials with control of colour and optical response on the nanoscale'. Another possibility is to isolate atoms with spin in the channels to act as quantum bits in memories or quantum information technologies.

'This system is actually a laboratory to study many physical, chemical and biological entities in nano-confinement,' says Boris Gorshunov of the Moscow Institute of Physics and Technology in Russia. Gorshunov also imagines studying ferromagnetic or ferroelectric behaviour of encapsulated atoms and molecules: recently he and co-workers reported ferroelectric alignment of water molecules in the channels of beryl.[2] 'This opens up a way to study exciting phenomena involving nano-caged entities,' he says.

Knut Urban, a physicist at the Jülich Research Centre in Germany, calls the result 'remarkable' and says that it might encourage more use of electron microscopy in mineralogy. 'The typical mineralogist is more used to x-ray scattering techniques. This work could unlock high-resolution [transmission electron microscopy]/Stem for mineralogy. If these methods are used by others in the future, there will be much more to come.'

Philip Ball

References

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2 B P Gorshunov *et al*, *Nat. Commun.*, 2016, **7**, 12842 (DOI: 10.1038/ncomms12842)

'Robo-chemist' optimises reactions in one day

Intelligent reactor drastically cuts time it takes to optimise cross-coupling reactions

Researchers in the US have developed an automated flow reactor that can respond to the results of experiments and determine the optimum conditions for catalytic reactions within a single day.

Identifying the ideal conditions for a catalytic reaction can be a laborious process: selecting the most efficient catalyst system in addition to assessing continuous variables like temperature, time and reagent concentrations can easily take hundreds of separate experiments.

Now, a team of chemists and chemical engineers led by Stephen Buchwald and Klavs Jensen from the Massachusetts Institute of Technology has developed a system that drastically cuts the time researchers spend optimising reactions. The hands-free approach identified optimum conditions within 96 experiments, each taking less than 10 minutes, for a series of Suzuki–Miyaura cross-couplings – important carbon–carbon bond forming reactions that are widely used in industry.

'The robotic system we present here conducts its own experiments, processes the data and uses the information it collects to select new experiments to optimise each reaction, similar to how a chemist would,' explains Brandon Reizman, who worked on the project.

The system uses an automated liquid handler to produce microlitre scale reaction droplets. These are pushed through a reactor and the resulting mixture separated and analysed. A computer algorithm then processes the results and feeds back instructions for the liquid handler to prepare the next reaction droplet.

'The algorithm looks at the shared relationships among both the discrete variables and continuous variables, like temperature and time, and then using those relationships it converges very quickly to where it thinks the best results might be,' explains Reizman.

Ryan Hartman, an expert in flow chemistry and microsystems based at New York University, US, lauds the research as a 'vital contribution that advances both synthetic chemistry and chemical engineering'. Commenting on the significance of the new system, he says that 'the automation of laboratory-scale reactors is one of the most important, yet challenging chemical engineering feats that could revolutionise the way we discover science in the 21st century'.

Jamie Durrani

Reference

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